# Perturbations of Noise: The Origins of Isothermal Flows

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**Abstract**

We make a detailed analysis of both phenomenological and analytic background for the "Brownian recoil principle" hypothesis (Phys. Rev. A 46, (1992), 4634). A corresponding theory of the isothermal Brownian motion of particle ensembles (Smoluchowski diffusion process approximation), gives account of the environmental recoil effects due to locally induced tiny heat flows. By means of local expectation values we elevate the individually negligible phenomena to a non-negligible (accumulated) recoil effect on the ensemble average. The main technical input is a consequent exploitation of the Hamilton-Jacobi equation as a natural substitute for the local momentum conservation law. Together with the continuity equation (alternatively, Fokker-Planck), it forms a closed system of partial differential equations which uniquely determines an associated Markovian diffusion process. The third Newton law in the mean is utilised to generate diffusion-type processes which are either anomalous (enhanced), or generically non-dispersive.

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# 1 Smoluchowski diffusion processes, Stokes resistance and weakly out-of-equilibrium systems

## 1.1 Traditional phenomenology

In random media that at are statistically at rest, motion of single tracers or dispersion of pollutants, also in the presence of external conservative force fields, may be consistently described in terms of Smoluchowski diffusion processes, [1, 2]. Their forward drifts are interpreted to give account of the mean velocity $\beta^{-1}\vec{F}/m$ imparted by the external conservative force to diffusing particles, an outcome of the acceleration $\vec{F}/m$ "felt" and accumulated on the relaxation time scale $\beta^{-1}$. This time scale is regarded to be much finer than the one appropriate for the coarse-grained description. The latter, $\triangle t \gg \beta^{-1}$, is still significantly smaller than the available phenomenological (observational) resolution.

Our basic intuitions are rooted in the theory of a Brownian motion suitable for the description of colloidal particles floating in a liquid. However an issue of particular "causes of diffusion" is not that relevant, and the proper arena for the Brownian motion can be not only a viscous fluid, or a dilute gas, but any interacting many-particle system and even less specific random medium with a suitable microscopic behaviour. The problem of "how to make a heat bath" needs to be addressed, [2, 3, 4]. In the present paper, we take for granted the validity (even if diminished to the status of an approximate theory or the conceptual playground) of the standard Kramers and Smoluchowski diffusion process scenarios, as the reference mathematical models of random transport in the equilibrium bath.

If we consider a fluid in thermal equilibrium as the noise carrier, a kinetic theory viewpoint amounts to visualizing the constituent molecules that collide not only with each other but also with the tagged (colloidal) particle, so *enforcing* its observed erratic motion. Clearly, random molecular collisions both initiate and maintain an incessant irregular motion of the tagged particle. Once the particle is in motion,

we need to account for an additional statistical effect of molecular impacts on the actually *moving* particle. It is phenomenologically encoded in the Stokes resistance, coming from averaging over a molecular "rain" along some portion of the trajectory, which is proportional to the velocity of the particle. In the phase-space description, the particle velocity $\vec{V}(t) = \vec{v}$ is a random quantity. The damping effect is *not* random. It stands for a statistically accumulated, passive response of the medium. Indeed (see e.g. Section 2.1 in below), $-\frac{\vec{v}}{\beta^{-1}}$ locally averages the genuine (ignored fine-detailed) random dynamics on the relaxation time scale $\beta^{-1}$.

For a bath in equilibrium, the internal relationship between the above random and systematic (due to friction) effects of a generic noise on the Brownian particle motion is the subject of fluctuation-dissipation theorems. This extends to situations when the external driving forces additionally modify the particle dynamics, but do not modify the statistics of noise (!). This feature is generic to Smoluchowski diffusions. (Conventionally, the fluctuation-dissipation theorems are interpreted, [5], to set a general relationship between the response of diffusig particles in an equilibrium bath to an external force, and the internal fluctuation of the bath in the absence of this disturbance.)

By means of Einstein's fluctuation-dissipation theorem we are given the diffusion coefficient $D = \frac{kT}{m\beta}$. It characterises an intensity of the spatial (Wiener) noise in terms of the friction parameter $\beta$, with $k$ the Boltzmann constant, $T$ the equilibrium temperature of the bath, and $m$ mass of a diffusing particle, [1]. A formal exploitation of the Stokes formula (derivable on the basis of pure kinetic arguments from the Boltzmann theory, [6]) transfers to the Brownian realm a concept of a frictional deceleration, originally suited for a macroscopic spherical particle of radius $a$ and mass $m$ moving in a fluid with viscosity coefficient $\eta$. In the new context, it is the *mean* property of motion and *not* a particular single Brownian particle-in-motion attribute. Nonetheless, that allows to establish the value of the friction constant $\beta = 6\pi\eta a/m$, the result amenable to positive experimental verifications in

the classic studies of the Brownian motion, [1, 7].

## 1.2 Meaning of stochastic models

An observable Brownian motion of colloidal particles in a fluid, [1, 7], when interpreted in terms of random processes, involves a number of mathematical subtleties, like e.g. an inherent nondifferentiability of sample paths in velocity space that reappears on the spatial arena of Smoluchowski processes as well.

Clearly, the phase-space stochastic process is rather crude approximation of reality, if compared with the kinetic theory reasoning based on the explicit input of particle collisions to the Boltzmann equation and the related kinetic theory of hydrodynamic flows, [6]. The Boltzmann equation can be interpreted in terms of a jump Markov process simulating collision events, and the diffusion-type Karmers equation may arise only in a suitable scaling limit, [8]. This limit can be justified in case of grazing collisions, or as a way to include the effect of long range forces by treating their influence in a statistical way: they should generically produce a sequence of small and almost random changes in the tracer particle velocity, [3].

The Smoluchowski *approximation* takes us further away from the kinetic theory intuitions by projecting the phase-space theory of random motions into its configuration space image, [9], which is a spatial Markovian diffusion process.

To quantify the above picture one usually departs from the phase-space (Langevin and Kramers) description of fluctuation phenomena. Let us consider an Itô equation (in its symbolic differential version) for infinitesimal increments of the velocity random variable, exhibiting the systematic frictional resistance:

$$d\vec{V}(t) = -\beta\vec{V}(t)dt + \beta\sqrt{2D}d\vec{W}(t) \tag{1}$$

where $\vec{W}(t)$ stands for the normalised Wiener process. One can easily infer, [10], the corresponding second Kolmogorov (Fokker-Planck) equation

$$\partial_t p(\vec{v}_0, \vec{v}, t) = \beta D \triangle_{\vec{v}} + \beta \nabla_{\vec{v}} \cdot [\vec{v}\, p(\vec{v}_0, \vec{v}, t)] \tag{2}$$

for the transition probability density of the time homogeneous process in the velocity space alone, [10, 2].

In view of:

$$p(\vec{v}_0, \vec{v}, t) = (\frac{m}{2\pi kT(1-e^{-2\beta t})})^{3/2} exp\{\frac{m}{2kT}\frac{(\vec{v}-\vec{v}_0 e^{-\beta t})^2}{1-e^{-\beta t}}\} \tag{3}$$

the time interval $\beta^{-1}$ effectively accounts for an approach of the transition density to the equilibrium Maxwell distribution.

Let us consider an instantaneous velocity $\vec{V}(t) = \vec{v}$, that has been achieved in the course of the random evolution (1) beginning from a certain $\vec{V}(0) = \vec{v}_0$. We can evaluate a conditional expectation value (local mean with respect to the law of random displacements (3)) over all randomly accessible velocities $\vec{V}(t+\triangle t) = \vec{v}'$ at a time $t+\triangle t$, $\triangle t > 0$. It determines the forward drift of the process:

$$\vec{b}(\vec{v}, t) = lim_{\triangle t \downarrow 0}[\int \vec{v}'\, p(\vec{v}, \vec{v}', \triangle t)\, d^3v' - \vec{v}] = -\beta\vec{v} \tag{4}$$

and thus, [2, 11, 12], provides us with an information about the *mean tendency* of the dynamics on small (but not too small if compared to $\beta^{-1}$) time scales. Evidently, that mean tendency in case of Eq. (1) is to decelerate the velocity $\vec{v}$ at the Stokes rate $\frac{\vec{v}}{\beta^{-1}}$.

Sample paths of the Wiener process are nondifferentiable and play the rôle of (velocity space) idealizations of "true" trajectories. We need a conditional averaging over all paths emanating from $\vec{v} = \vec{V}(t)$ to bypass, cf. Eq.(4), the nondifferentiability problem and then introduce the local deceleration rate ($\vec{v} \to \vec{v} - \beta\vec{v}\triangle t$), [2]. Clearly, the friction term and thus the deceleration concept, in the framework set by Eq. (1), arise as statistical, *local mean value*, quantities. All that must be sharply contrasted with the standard hydrodynamical meaning of the Stokes resistance formula, which refers to a genuine (the reduced Navier-Stokes equation is involved) fluid velocity field around a *single* uniformly propagating particle. It is the perturbation by the moving macroscopic body that gives rise to the force, with which the viscous fluid acts upon the concrete particle-like object.

Quite apart from the time-scale ($\triangle t$ versus $\beta^{-1}$) issue, an individual Brownian particle neither moves uniformly, nor *ever* permanently relaxes to the state of rest. Actually, for a single Brownian particle, the respective velocity gain/loss (acceleration/deceleration rate) on the $\beta^{-1}$ time scale *is a random quantity.*

On the contrary, the standard interpretation of the Stokes resistance for a large particle in a viscous fluid, makes inavoidable an ultimate stopping of the particle, unless an external force would balance the damping and so maintain the (uniform) particle motion at a certain terminal velocity. This latter concept forms the basis of the Einstein fluctuation-dissipation formula in case of the gravitationally induced sedimentation phenomenon, cf. [1], albeit in case of the Brownian motion only local mean velocity fields (hence, ensemble averages) can be employed for that purpose. The picture of "a Brownian particle moving at its terminal velocity", [13], is certainly inappropriate.

We can supplement Eq. (1) by the spatial increment definition: $d\vec{X}(t) = \vec{V}(t)dt$, extending (1) to the phase-space process whose Smoluchowski projection in the large damping regime reduces to the pure spatial Wiener noise $d\vec{X}(t) = \sqrt{2D}d\vec{W}(t)$. In this case, the generic spatial scale (wandering distance over which the dissipation process *in the mean* is completed) is set by $(D\beta^{-1})^{1/2}$. The Smoluchowski approximation amounts to ignoring the fine details of the dynamics on the $\beta^{-1}$ and $(D\beta^{-1})^{1/2}$ scales. One disregards all possible remnants of the phase space process that extend beyond those scales (the damping typically induces $exp(-\beta t)$ factors in all relevant formulas, hence a certain amount of "memory" must be eliminated to yield a Markov process), [1].

That particular *disregard/ignore* issue is worth emphasizing in the context of typical approximate (analytic or numerical) manipulations with the Brownian motion. A strong solution of Eq. (1) (we take $\vec{V}(0) = \vec{v}_0$ as the initial condition) has the form :

$$\vec{V}(t) = \vec{v}_0 exp(-\beta t) + \int_0^t exp[-\beta(t-s)]\sqrt{2D}d\vec{W}(s) \ . \tag{5}$$

This expression, albeit looking physically unrealistic, is a fairly accurate approximation of a phenomenological molecular collision scenario for the Brownian motion. Namely, let us introduce a finite Riemann sum approximation of the integral in Eq. (5):

$$\int_0^t exp[-(t-s)]\sqrt{2D}d\vec{W}(s) \approx exp(-\beta t)\sum_n exp(\beta n\triangle t)\triangle\vec{V}_n \qquad (6)$$

where $\triangle\vec{V}_n = \sqrt{2D}\triangle\vec{W}(n\triangle t)$ stands for the n-th consecutive velocity increment, e.g. an effect of all "random acceleration" events taking place in the time interval $(n\triangle t, (n+1)\triangle t)$. If we resort to a molecular collision mechanism (in a dilute gas for example), the velocity increments due to collisions of the Brownian particle with molecules of the bath can be viewed as statistically independent, and occur at an approximate rate $10^{-21}$ per second. The collisions may be interpreted to occur consecutively one after another, but multiple collision events are allowed as well. If we regard the time coarse-graining in Eq. (6) to refer to a typical relaxation time $\beta^{-1} \approx 10^{-8}s$, (notice that the respective coarse-graining appropriate for the Smoluchowski approximation, would involve $\triangle t \gg \beta^{-1}$), it is obvious that each n-th velocity increment can be interpreted as a sum of an enormous number of independent identically distributed random variables (minute acceleration/deceleration, e.g. collision events). Let us stress that we exploit here a defining property of the Wiener process; the velocity random variable (5) of the Ornstein-Uhlenbeck process (1)-(3) is known *not* to have independent random increments, [10].

The accumulated fluctuation irregularities, on the $\beta^{-1}$ time scale, are the primary reason of the erratic behaviour of the Brownian motion in the velocity space. Thus, an integration with respect to the normalised Wiener process $\vec{W}(t)$ in Eq. (5), quite satisfactorily (in a suitable scaling limit) models a *cumulative* outcome of phenomenologically motivated impulses (kicks exerted by the noise carrier) on the Brownian particle.

Let us emphasize at this point, [2], that it is not correct to think that conspicuous jiggles in the Brownian trajectory are due to *single* kicks. (In mathematical terms

the situation is even worse, since the Wiener process has an unbounded variation on aritrary time intervals.) The realistic Brownian motion is unbelievably gentle, specifically if we refer to a heavy particle immersed in a gas of much lighter ones. Each collision (kick) has an entirely negligible effect on the velocity of the Brownian particle. It is only fluctuations in the accumulation of an enormous number of very slight changes in the particle velocity which give the trajectory its irregular appearence, both in velocity and position pictorial representations of motion. Conequently, equation (5) makes sense as a useful approximation of physical phenomena, if the coarse-grained time scale $\triangle t$ in (6) (which is far below an observational one) is much larger than $\beta^{-1}$, but still small enough for a sufficiently fine coarse-graining (6) of (5).

The previously mentioned space and time scales justify the utility of the Smoluchowski description of conservative force effects upon a spatially diffusing particle, [2]:

$$d\vec{X}(t) = \frac{\vec{F}}{m\beta}dt + \sqrt{2D}d\vec{W}(t) \ . \tag{7}$$

The Smoluchowski forward drift can be traced back to a presumed selective action of the force on the Brownian particle that has a negligible effect on the thermal bath. Indeed, we take for granted that there is no physically relevant mean (induced) flow in the bath proper, unless the isothermality assumption is abandoned, [13, 14], or other hitherto disregarded effects on the $\beta^{-1}$ scale (like those due to the action-reaction principle, [11]) are incorporated into the formalism.

Brownian particles appear to be drifting *on the local average* relative to the bath, with a uniform (but in the mean !) velocity $\frac{\vec{F}}{m\beta}$. Clearly, a repeated series of observations, at regularly spaced time intervals, of a *single* tagged Brownian particle would not in general reveal any specific motion tendency. The graphical picture of motion would be as irregular as ever ("no purpose" sample paths of the Wiener process, like in the absence of any force). The respective coarse-grained approximation of the trajectory does correspond to an experimental resolution, which is incomparably

rougher than the previous time scales.

Only a numerical simulation of the statistical ensemble of sample paths with a controlled probability distribution (frequency, in fact) of initial conditions, or a realistic monitoring of the Brownian motion-induced dispersion of a low density cloud of dust particles suspended in a liquid, would lend a definite meaning to the "motion tendency" concept and to the related mean Brownian flows. Realistic diffusion processes (and diffusive transport) are observed in case of non-uniform concentrations of colloidal particles but they are regarded as a result of random migration of individual particles which is actually observable (under a microscope) and interpreted as the Brownian motion.

In the context of a sedimentation phenomenon, a sufficiently long overall observation time of a single tagged particle travelling along its erratic path (hours or days in a real, or computer simulation experiment), would presumably reveal that a particle more frequently visits certain spatial areas, in accordance with the barometric formula (ergodic features of motion). Early experiments on this issue, [1, 7], pertained to a cloud of suspended particles executing an extremely slow (practically adiabatic) diffusion process. In some cases, the spatial displacement of the size $0.2 \cdot 10^{-6}m$ tracer particles has been measured in $30s$ time intervals, [7, 1], to yield the observationally relevant outcomes. Very recent observations of an individual Brownian particle motion refer to $1 - 2.5 \cdot 10^{-6}m$ tracers and the $\frac{1}{60}s$ time resolution.

## 1.3 Problems with thermal equilibrium

A spectacular solution of the sedimentation problem due to Smoluchowski, refers to the isothermal dynamics (1) which is constrained to the positive vertical semiaxis: $dZ(t) = -\beta c dt + \beta\sqrt{2D}dW(t)$, with a reflecting boundary at the spatial point 0. The transition probability density of this one-dimensional process reads, [1, 10]:

$$p(z, z_0, t) = \frac{1}{2(\pi Dt)^{1/2}}\{exp[-(z - z_0)^2/4Dt] + exp[-(z + z_0)^2/4Dt]\}+$$

$$\frac{c}{D\sqrt{\pi}} exp(-cz/D) \int_{\frac{z+z_0-ct}{2(Dt)^{1/2}}}^{\infty} exp(-x^2)dx \tag{8}$$

and shows that a particle starting its motion from any positive $z_0$ near 0, may wander along the positive semiaxis indefinitely. In particular, it can be transported against the gravitational force to an arbitrary height. Depending on the actual $z_0$ the Brownian particle may have a higher probability to ascend than to descend.

The corresponding *mean work* has been evaluated to be $kT$ per particle, cf. [1, 10] for a related discussion of the entropy decrease issue. Certainly, an ability of the medium to perform work (in the mean) i. e. to give a kinetic energy to the Brownian particle (on the ensemble average again), is not special to the sedimentation problem. It appears to be a universal feature of the thermal bath even in the absence of any external forces.

In the equilibrium situation ($t \to \infty \Rightarrow p(z, z_0, t) \to \rho(z)$), we would arrive at the familiar balance condition: the mean tendency of motion (forward drift) due to gravitational acceleration must be exactly balanced by the oppositely directed motion tendency of the diffusive (osmotic pressure, [1, 2]) origin, valid for non-uniform concentrations of a contaminant in a solvent. The latter tendency involves sending particles away from the areas of higher probability of their presence (concentration, if a low density pollutant is considered) in accordance with the Fick formula for the diffusion current $-c = -D\frac{\nabla\rho(z)}{\rho(z)}$. The barometric formula does follow.

It is interesting to spend a while on some tagged (single) particle features in the nonequilibrium–but isothermal–regime admitted by (8) for not too large times, when the Einstein (mean) balance condition is yet invalid. Clearly, to have defined an analogue of the Fick diffusion flow, a probability density of initial data $z_0$ must be chosen. In a computer simulation we would have under control a bunch of relevant sample paths (all consecutively executed on a fixed duration time interval $[0, t]$) and the related probability density evolution along the bunch. Depending on the initial data distribution, for a time period the osmotic drift would dominate the gravitationally induced drift. To this end, work (in the mean) must have been done

on Brownian particles *at the expense of the bath.* Local conversion of work into heat seems to be inavoidable, and local heat flows are inavoidable as well, cf. [13, 7]. That creates a number of problems to which no attention is normally paid in the literature.

Smoluchowski diffusions are conventionally regarded as isothermal processes (possible heat flows are ignored by various reasons). If we however admit that the emerging tiny heat flows may have an affect on the particle transport due to the Brownian motion, a suitable description of the thermal inhomogeneities and their effects on the dispersion of Brownian particles must be invented.

For example, in case of thermally inhomogeneous gases it is well known that a dust-free region appears about a hot body, showing that a temperature gradient has an effect on the motion of dust particles in a gas, [16]. Tracer particles are transported away from the hot areas to the cooler ones (we may interpret that as a repulsion by the heated domain). On the reverse, they appear to be attracted by the cooler areas while escaping from the hot domains. Particles float down the temperature gradients.

**Remark 1:** Let us mention an approach to quite similiar problem, [13] which was originally formulated for a cloud of contaminants in a liquid, under the following phenomenological assumption: "a gas of Brownian particles falling in gravity should leave a trail of warm fluid in its wake, since its potential energy is being converted into heat". Obviously, if the particles would move against gravitational force, then the temperature of the medium should locally drop down. Those features, if we are to keep track of the local heating and cooling (as opposed to the isothermal Einstein or Smoluchowski diffusive dynamics) were interpreted as a source of the space-time dependence of temperature. The Fokker-Planck equation must then be supplemented by an evolution equation for the temperature field, (a clear-cut kinetic theory reasoning can be read out in this strategy), so that the coupled nonlinear system would take the form of a "consistent thermodynamical system" i. e. the

one manifestly respecting the first and second laws of thermodynamics, see e. g. Ref. [14]. Here, the heat flows are assumed to be neither slow nor fast enough to be effectively disregarded.

**Remark 2:** An issue of suitable slow and fast process time scales is crucial in our discussion. One should be aware that local temperature perturbations of the bath may be safely neglected when the dissipation (fast process) time scale and the diffusion (observational for tagged particles) time scales are generically incompatible, like e.g. in case of a rapid dissipation set against a slow diffusion process. Then, the usual isothermal diffusion process follows and the standard Brownian motion paradigm is left intact.

In the discussion of the Carnot principle, in reference to the free Brownian motion and to the sedimentation problem, [1, 7], Brownian particle fluctuations are regarded to occur due to causes that are intrinsic to the random medium. If we think about minute acceleration/deceleration events that modify (say, at a rate of $10^{21}$ times per second) velocities of realistic particles, the microscopic energy-momentum conservation laws need to be respected in each separate collision event. In contrast to derivations based on the Boltzmann colllision scenario, this feature is completely *alien* to the Brownian motion theory, cf. [11, 12]. (This happens quite apart from the elusive power of the flutuation-dissipation mechanism, [5]: "The friction, or more generally the resistance of a given system, represents the method by which the external work is dissipated into microscopic thermal energy. The reverse process is the generation of random force as the result of thermal fluctuation".)

Let us point out that the phenomenology allowing to regard Eq. (1) as a satisfactory model for Brownian particle velocity fluctuations, blurs possible advantages of the closely related argument appearing in the diffusion modeling of the Raileyigh piston, [17]: " Collisions between the large particle (piston) and the bath particles are elastic. After each collision the bath particles are given a new distribution, which

evolves until the next collision".

To avoid an apparent contradiction with the law of energy conservation, there seems tempting to require that each minute acceleration of a Brownian particle is accompanied by a minute *cooling* of the medium in its immediate neighbourhood. Correspondingly, any deceleration event should induce a local *heating* of the immediate neighbourhood of a particle, see e.g. [7]. Since (cf. Eq. (1)), we always disregard the fine details of about $10^{13}$ collision impacts on the Brownian particle on a typical relaxation time scale of $10^{-8}s$, there is definitely enough room to allow for local statistical measures of heating and cooling.

**Remark 3:** The heating, cooling and temperature notions are quantitative mean measures of the degree of agitation of the noise carrier. If the random medium is interpreted on the molecular level to be composed of light particles, these measures can be related with the mean square deviation of the (bath molecule) velocity random variable, or an average of the squared velocity if its mean value vanishes. Those quanties are purely statistical characteristics of the bath and *not* of the Brownian particle immersed in it. Only under restrictive thermal equilibrium conditions, the notion of temperature appropriate to the bath, can be elevated to the status of a measure of a thermal agitation for tracer particles.

## 1.4 Goals

In the Kramers approach to the phase-space dynamics, the stochastic properties of the medium were considered to be independent from random phase-space data of the Brownian particle. The statistics of noise (e. g. the thermal equilibrium features of the bath) must have remained unperturbed by the very presence of the particle and its phase-space fluctuations, albeit those are *enforced* by the intrinsic randomness of the bath. One assumes that there is no relevant *dynamical* response of the bath to the very presence of the Brownian particle and its induced dynamics. We recall that the fluctuation-dissipation theorems merely account for a *passive*

response, in terms of the statistically implemented Stokes resistance of the bath to the particle-in-motion.

On the other hand, the above local heating and cooling notions refer to the dynamical response of the bath to the Brownian particle which is immersed in it. We need to account for the out-of-equilibrium properties of the bath in the presence of a single particle, whose motion is solely enforced by the bath. Thus very weak (although possibly fast) heat flows should accompany an individual Brownian particle motion. That conforms with an obvious intuition that no physical system is ever in thermodynamical equilibrium, and normally it is necessary to idealize the situation by regarding "fast processes" to be completed, while the "slow" ones are still running.

In such a weakly non-equilibrium system with small heat flows, we may expect that the standard equilibrium temperature notion is replaced by an *effective* temperature notion (and an effective thermal equilibrium), which depends on the chosen fast-versus-slow-process time scales and the ensemble averaging. Repetitions of a single particle experiment in the same thermal bath, should now be replaced by repetitions of the same experiment with different realizations of the out-of-equilibrium heat bath, cf. [18] for similiar concepts in the context of randomly disordered media.

In the above sense only an effective isothermal regime may be maintained, since the compensating heat flows allow to regain the equilibrium temperature *almost* instantaneously. After averaging over the tracer particle ensemble and the corresponding (weakly out-of-equilibrium) sample paths, we should be able to capture possible statistically relevant effects due to temperature inhomogoneities (small deviations from thermal equilibrium conditions) and the resultant effective flows *in a bath,* that are possibly induced (via back reaction on the time scale probably larger than $\beta^{-1}$ but still much below the Smoluchowski approximation time scale $\triangle t$) by propagating Brownian particles. All that is to happen well beyond the limits of an available, cf. [7], observational resolution.

We have thus set a phenomenology of a specific *dynamical* response of the random medium to the Brownian motion of a *single* tagged particle, whose sole outcome are the minute deviations from the thermal equilibrium of the fluctuating medium itself and the resultant heat flows (needed to restore the equilibrium). This is independent from the traditional frictional resistance argument, directly referring to the thermal equilibrium conditions and the $\beta^{-1}$ time scale.

We deal here with a generic *feedback mechanism* scenario. The Brownian particle propagates "at the expense" of the bath, which however remains "close" to its thermal equilibrium. The bath in turn actively *reacts back* to what is being happenning to the particle in the course of its propagation. The instantaneous local deviations from the state of equilibrium ("perturbation of noise") along the trajectory surely have an effect on each subsequent stage of the particle propagation. Even if residual for an individual Brownian particle and its sample path, the feedback effect is expected to accumulate statistically (on the ensemble average) to a sizable quantity. Under the name of the "Brownian recoil principle" we have made a preliminary study of such random dynamics in Refs. [11, 12].

**Remark 4:** In connection with the previous Remark 1, let us mention that a spatial diffusion (Smoluchowski) approximation of the phase-space process, allows to reduce the number of independent local conservation laws (cf. [15, 19, 20]) to two only. Therefore the Fokker-Planck (or continuity) equation can always be supplemented by another (independent) partial differential equation to form a closed system. Non-isothermal flow description needs to accomodate the variations of temperature of the bath, (cf. [13, 14]), while we investigate the limits of validity of the isothermal scenario. That amounts to inequivalent choices of the supplementary equation. We emphasize a single tagged particle-in a bath description in a repeatable experimentation sequence, under basically the same (or very similiar) physical conditions. In such situation, a stochastic process executed by a single particle is practically isothermal ("the Brownian motion is unbelievably gentle", [2]). Each

sample path of the Brownian particle (and the related cooling/heating phenomena induced along the path) is a random quantity. The state of the medium, if giving account of its *dynamical response* (i. e. deviation from thermal equilibrium) to the Brownian propagation, is a random quantity as well. It is the local mean (related to the ensemble average over various realisations of out-of-equilibrium conditions for the bath) that may properly quantify this picture.

# 2 Local conservation laws for the Brownian motion in the Smoluchowski approximation: diffusion currents and driving flows

Before, we have identified the forward drift $\frac{\vec{F}}{m\beta}$, $\vec{F} = -\vec{\nabla}V$ as a quantitative measure of a statistical (local) tendency of the Brownian motion, obtained through averaging over an ensemble of sample paths. If we assign a probability density $\rho_0(\vec{x})$ with which the initial data $\vec{x}_0 = \vec{X}(0)$ for Eq. (7) are distributed (weak solutions of (7) enter the scene), then the emergent Fick law would reveal a statistical tendency of particles to flow away from higher probability residence areas. This feature is encoded in the corresponding Fokker-Planck equation (equivalently, a continuity equation):

$$\partial_t \rho = -\vec{\nabla} \cdot (\vec{v}\rho) = -\vec{\nabla} \cdot [(\frac{\vec{F}}{m\beta} - D\frac{\vec{\nabla}\rho}{\rho})\rho] \tag{9}$$

where a diffusion current velocity is $\vec{v}(\vec{x},t) = \vec{b}(\vec{x},t) - D\frac{\vec{\nabla}\rho(\vec{x},t)}{\rho(\vec{x},t)}$ while the forward drift reads $\vec{b}(\vec{x},t) = \frac{\vec{F}}{m\beta}$, cf. Eq. (7). Clearly, the local diffusion current (a local flow that might be experimentally observed for a cloud of suspended particles in a liquid) $\vec{j} = \vec{v}\rho$ is nonzero in the nonequilibrium situation and a non-negligible matter transport occurs as a consequence of the Brownian motion, on the ensemble average.

It is interesting to notice that the local velocity field $\vec{v}(\vec{x},t)$ obeys the natural (local) conservation law, which we quite intentionally pattern after the moment

identities (hierarchy of conservation laws) valid for the Boltzmann and Kramers equations, [9, 15]. The pertinent momentum conservation law directly originates from the rules of the Itô calculus for Markovian diffusion processes, [2], and from the first moment equation in the diffusion approximation (!) of the Kramers theory, [9, 15]:

$$\partial_t \vec{v} + (\vec{v} \cdot \vec{\nabla})\vec{v} = \vec{\nabla}(\Omega - Q) \ . \tag{10}$$

An effective potential function $\Omega(\vec{x})$ can be expressed in terms of the forward drift $\vec{b}(\vec{x}) = \frac{\vec{F}(\vec{x})}{m\beta}$ as follows:

$$\Omega = \frac{\vec{F}^2}{2m^2\beta^2} + \frac{D}{m\beta}\vec{\nabla} \cdot \vec{F} \ . \tag{11}$$

Let us emphasize that it is the diffusion (Smoluchowski) approximation, [9, 15], which makes the right-hand-side of Eq. (10) substantially different from the usual moment equations appropriate for the Brownian motion, [15]. In particular, the force $\vec{F}$ presumed to act upon an individual particle, does not give rise in Eq. (10) to the expression $-\frac{1}{m}\vec{\nabla}V$ which might be expected on the basis of kinetic theory intuitions and moment identities directly derivable from the Karmers equation, but to the term $+\vec{\nabla}\Omega$, cf. Eq. (11).

Moreover, instead of the standard pressure term, there appears a contribution from a probability density $\rho$-dependent potential $Q(\vec{x}, t)$. It is is given in terms of the so-called osmotic velocity field $\vec{u}(\vec{x}, t)$, (cf. [2]):

$$Q(\vec{x}, t) = \frac{1}{2}\vec{u}^2 + D\vec{\nabla} \cdot \vec{u} \tag{12}$$

$$\vec{u}(\vec{x}, t) = D\vec{\nabla}\, ln\rho(\vec{x}, t)$$

and is generic to a local momentum conservation law respected by isothermal Markovian diffusion processes, cf. [2, 11, 12, 19]. Notice that in case of the free Brownian motion (admitted, if we set $\Omega = 0$), we would have $\vec{v}(\vec{x}, t) = -\vec{u}(\vec{x}, t)$ for all times.

An equivalent form of the potential (12): $Q = 2D^2\frac{\triangle\rho^{1/2}}{\rho^{1/2}}$ induces rather obvious quantum mechanical associations (the de Broglie-Bohm "quantum potential" with

the opposite sign, modulo an adjustment of constants), [21]. In the context of the Brownian motion, this "quantum potential" has been deduced in earlier investigations of local conservation laws, [20].

**Remark 5:** Let us notice that by demanding $Q = \Omega$ identically for all $\vec{x}, t$, we would reduce Eq. (10) to $\partial_t \vec{v} + (\vec{v} \cdot \vec{\nabla})\vec{v} = 0$. Despite of its classical-looking Riemann equation form, this conservation law still refers to a diffusion process. Namely, in view of (11), we must identify forward drifts with osmotic velocity fields and $D\vec{\nabla} ln\, \rho(\vec{x}) = \frac{\vec{F}}{m\beta}$ holds true. The related diffusion process is stationary and preserves the probability measure ($\rho$ is now time-independent). Cf. [22] for more general considerations on that issue.

As repeatedly stated before, Smoluchowski drifts refer to mean motions relative to the bath at rest, and there is no place for any flows intrinsic to the random medium in this formalism. On the other hand, it is of fundamental importance to understand how genuine flows in a random medium may be generated and what would be their effect on dispersion, [12]. (Solutions of the incompressible Navier-Stokes equation may serve as a common-sense model of the flow in a bath, and the diffusion enhancement is known to be related to various turbulent motion scenarios.)

To analyze random perturbations that are either superimposed upon or are intrinsic to a driving deterministic motion, a configuration space equation $\dot{\vec{x}} = \vec{w}(\vec{x}, t)$ is normally invoked, which is next replaced by a formal infinitesimal representation of an Itô diffusion process

$$d\vec{X}(t) = \vec{b}(\vec{X}(t), t)dt + \sqrt{2D}d\vec{W}(t) \tag{13}$$

patterned after Eq. (7). The tacit assumption (basically wrong, [23]) is that $\vec{b}$ does not substantially differ from $\vec{w}$.

It is useful to exploit a standard phase-space argument that is valid, under isothermal conditions, for a Markovian diffusion process taking place in (or relative to) a flow $\vec{w}(\vec{x}, t)$ with as yet unspecified dynamics nor concrete physical origin. We

account for an explicit force (here, acceleration $\vec{K} = \vec{F}/m$) exerted upon diffusing particles, while not directly affecting the driving flow itself. Namely, [10, 2], let us set for infinitesimal increments of phase-space random variables:

$$d\vec{X}(t) = \vec{V}(t)dt$$

$$d\vec{V}(t) = \beta[\vec{w}(\vec{x},t) - \vec{V}(t)]dt + \vec{K}(\vec{x})dt + \beta\sqrt{2D}d\vec{W}(t) \ . \tag{14}$$

Following the leading idea of the Smoluchowski approximation, we assume that $\beta$ is large, and consider the process on time scales significantly exceeding $\beta^{-1}$ (that is normally achieved by taking $\beta$ to be very large, cf. the infinite friction limit procedure). Then, an appropriate choice of the velocity field $\vec{w}(\vec{x},t)$ may in principle guarantee, [2], the convergence of the spatial part $\vec{X}(t)$ of the process to the Itô diffusion process with infinitesimal increments :

$$d\vec{X}(t) = [\vec{w}(\vec{x},t) + \frac{1}{\beta}\vec{K}]dt + \sqrt{2D}d\vec{W}(t) \ . \tag{15}$$

Consequently, the forward drift of the process would read $\vec{b}(\vec{x},t) = \vec{w}(\vec{x},t) + \frac{1}{\beta}\vec{K}(\vec{x})$. Notice that the $\beta^{-1}\vec{K}$ contribution can be safely ignored if we are interested in the dominant driving motion.

Throughout the paper we are interested in Markovian diffusion processes, which propagate respectively the phase-space or configuration space probability densities (weak solutions of stochastic differential equations are thus involved). In the configuration space variant corresponding to Eqs. (13), (15), we deal with a stochastic process whose probability density $\rho(\vec{x},t)$ evolves according to the standard Fokker-Planck equation

$$\partial_t\rho = D\triangle\rho - \vec{\nabla}\cdot(\vec{b}\rho) \tag{16}$$

which is supplemented by the momentum conservation law (in the mean) of the form (10) for $\vec{v} = \vec{b} - D\frac{\vec{\nabla}\rho}{\rho}$. If we compare Eq. (15) with Eq. (7), we realize that the transformation of drifts has been executed. Under suitable restrictions, we can relate probability measures corresponding to those equations by means of the

Cameron-Martin-Girsanov theory of measure transformations. The Radon-Nikodym derivative of measures is here involved and for suitable forward drifts that are gradient fields it yields, [12], the most general form of an auxiliary potential $\Omega(\vec{x},t)$ that is allowed to appear in Eq. (10):

$$\Omega(\vec{x},t) = 2D[\partial_t\phi + \frac{1}{2}(\frac{\vec{b}^2}{2D} + \vec{\nabla}\cdot\vec{b})] \ . \tag{17}$$

Here $\vec{b}(\vec{x},t) = 2D\vec{\nabla}\phi(\vec{x},t)$.

Eqs. (17) and (11) are trivial identities, if we take for granted that all drifts are known from the beginning, like in case of typical Smoluchowski diffusions where the external force $\vec{F}$ is a priori postulated. We can proceed otherwise and, on the contrary, one can depart from a suitably chosen space-time dependent function $\Omega(\vec{x},t)$. Then Eq. (16) should be considered as a nonlinear (Riccatti-type) equation which is to be solved with respect to the drift field potential $\Phi(\vec{x},t)$. Such solution, when inserted to the Fokker-Planck equation (16) would ultimately yield an evolution of an initial probability density $\rho(\vec{x},0)$.

From this point of view, while developing the formalism, one should decide what is a quantity of a *primary* physical interest: the field of drifts $\vec{b}(\vec{x},t)$ or the potential $\Omega(\vec{x},t)$. They are not independent quantities, and enter the discussion as entangled objects. Mathematical features of the formalism appear to depend crucially on the properties (like continuity, local and global boundedness, Rellich class) of the potential $\Omega$, see e.g. [12].

If we decide that the momentum conservation law is governed by a bounded from below, continuous function $\Omega(\vec{x},t)$, cf. [12]), then it seems worthwhile to mention a close connection of the considered framework with the general theory of small random perturbations of the classical Hamilton-Jacobi dynamics, [19]. An assumption that the forward drift is defined in terms of a gradient of a suitable function allows to rewrite the formula (17) in the form clearly reminiscent of the Hamilton-Jacobi equation (we set $\Phi = 2D\phi$ in Eq. (17) and take $\Phi(\vec{x},0)$ as the

initial data for the $t \geq 0$ evolution):

$$\Omega = \partial_t \Phi + \frac{1}{2}|\vec{\nabla}\Phi|^2 + D\triangle\Phi \ . \tag{18}$$

An associated function (known as the so-called backward drift of a Markovian diffusion process) $\vec{b}_* = \vec{b} - 2\vec{u}$, cf. Eq. (11), if denoted $\vec{b}_* = \vec{\nabla}\Phi_*$ is known to yield another modified Hamilton-Jacobi equation, [12, 19]:

$$\Omega = \partial_t \Phi_* + \frac{1}{2}|\vec{\nabla}\Phi_*|^2 - D\triangle\Phi_* \tag{19}$$

to be solved with given terminal data $\Phi_*(\vec{x}, T)$ for times $0 \leq t \leq T$.

Eq. (19) is identifiable as the so-called Hamilton-Jacobi-Bellmann programming equation in the optimal control of stochastic diffusion processes, [19]. A related issue of viscosity solutions of the standard Hamilton-Jacobi equation has been extensively studied in the literature as the $D \downarrow 0$ limit of solutions of the modified (e.g. Bellmann) equation. A direct connection (via the logarithmic Hopf-Cole transformation) of Eq. (19) with the forced Burgers equation and the generalised heat equation (hence, with the related Feynman-Kac potentials, semigroups and kernels) is well known, [12, 19, 23].

There is however more interesting to observe that a gradient field ansatz for the diffusion current velocity ($\vec{v} = \vec{\nabla}S$):

$$\partial_t \rho = -\vec{\nabla} \cdot [(\vec{\nabla}S)\rho] \tag{20}$$

allows to transform the momentum conservation law (10) of a Markovian diffusion process to the universal Hamilton-Jacobi form:

$$\Omega = \partial_t S + \frac{1}{2}|\vec{\nabla}S|^2 + Q \tag{21}$$

where $Q(\vec{x}, t)$ was defined before in Eq. (12). By applying the gradient operation to Eq. (20) we recover (10). Notice that Eq. (20) is sensitive to any additive (constant or time-dependent) modification of the potential $\Omega$. In the above, the contribution

due to $Q$ is a direct consequence of an initial probability measure choice for the diffusion process, while $\Omega$ via Eq. (17) alone does account for an appropriate forward drift of the process.

The derivation of a hierarchy of local conservation laws (moment equations) for the Kramers equation can be patterned after the standard procedure for the Boltzmann equation, [6, 9, 15]. Those laws do not form a closed system and additional specifications (like the familiar thermodynamical equation of state) are needed to that end. In case of the isothermal Brownian motion, when considered in the large friction regime (e.g. Smoluchowski diffusion approximation), the Fokker-Planck equation must be supplemented by one conservation law *only* to yield a closed system. Such system uniquely determines the stochastic process.

That happens under a definite choice of external forces, and hence Smoluchowski drifts. If the drifts are not a priori specified, then the only freedom left in the momentum conservation law amounts to the choice of a concrete functional form for the potential $\Omega(\vec{x}, t)$. In the theory of Brownian motion this particular decision making replaces the standard equation of state constraint, suitable for the kinetic theory description of gases and liquids.

In view of more sensitive dependence on the potential and hence more detailed discrimination between distinct dynamics scenarios, we adopt the Hamilton-Jacobi equation (21) as a generic substitute of the momentum conservation law (10). Thus, we can consider a closed system which is composed of the continuity equation $\partial_t \rho = -\vec{\nabla}(\vec{v}\rho)$ (this, in view of $\vec{v} = \vec{b} - D\frac{\nabla\rho}{\rho}$, is equivalent to the Fokker-Planck equation (16)) and the Hamilton-Jacobi equation (21), plus suitable initial (and/or boundary) data. Alternatively, we can supplement the Fokker-Planck equation (16) by the nonlinear Riccatti-type equation (17) to form a closed system of partial differential equations, provided the functional form of $\Omega$ is pre-selected. In contrast to the pair (16), (21) where $\rho(\vec{x}, t)$ enters an entangled relationship, the pair (16), (17) is not entangled.

We need to stress that it is the closed system of Eqs. (20) and (21) which directly refers to physically motivated local conservations laws (moment equations) associated with the Brownian motion, [20, 15, 12], and to the respective diffusion currents. The underlying Markovian diffusion process is then specified *uniquely* (that would *not* be the case if (10) has been used instead of (21)). However, Eqs. (20) and (21) form a coupled nonlinear system, whose analytic solutions are not readily accessible. It is therefore useful to know that a *linearisation* of this formidable nonlinear problem is provided by a time-adjoint pair of generalised diffusion equations (cf. the Appendix) in the framework of the Schrödinger boundary data problem. The standard heat equation appears as a very special case in this formalism.

# 3 The third Newton law in the mean

## 3.1 Free Brownian motion in terms of local conservation laws

The local conservation law (10) acquires a direct physical meaning (the rate of change of momentum carried by a locally co-moving with the flow volume, [12]), only if averaged with respect to $\rho(\vec{x},t)$ over a simply connected spatial area. Namely, if $V$ stands for a volume enclosed by a two-dimensional outward oriented surface $\partial V$, we define a co-moving volume on small time scales, by deforming the boundary surface in accordance with the local current velocity field values. Namely, we consider at time $t$ the displacement of the boundary surface $\partial V(t)$ defined as follows: $\vec{x} \in \partial V \rightarrow \vec{x} + \vec{v}(\vec{x},t)\triangle t$ for all $\vec{x} \in \partial V$. Up to the first order in $\triangle t$ this guarantees the conservation of mass (probability measure) contained in $V$ at time $t$ i. e. $\int_{V(t+\triangle t)} \rho(\vec{x}, t+\triangle t)d^3x - \int_{V(t)} \rho(\vec{x},t)d^3x \sim 0$.

The corresponding (to the leading order in $\triangle t$) quantitative momentum rate-of-change measure reads, cf. [12], $\int_V \rho\vec{\nabla}(\Omega - Q)d^3x$. In view of $\partial_i Q = \frac{1}{\rho}\sum_j \partial_j P_{ij}$, where the stress tensor $P_{ij} = D^2\rho\partial_i\partial_j \, ln\, \rho$ is determined up to an additive time-dependent or constant term, the standard divergence theorem allows to isolate an

explicit surface (due to stresses or of the pressure-type) contribution. Namely, there holds $-\int_V \rho\partial_i Q d^3x = -\int_{\partial V}\sum_j P_{ij}d\vec{\sigma}_j$, with $d\vec{\sigma}$ being an infinitesimal area element of $\partial V$ in $R^3$.

For a particular case of the free Brownian expansion:

$$\rho_0(\vec{x}) = \frac{1}{(\pi\alpha^2)^{3/2}}exp(-\frac{x^2}{\alpha^2}) \rightarrow \rho(\vec{x},t) = \frac{1}{[4\pi D(t+t_0)]^{3/2}}\, exp[-\frac{\vec{x}^2}{4D(t+t_0)}] \quad (22)$$

where $\alpha^2 = 4Dt_0$ and $t_0 > 0, t \geq 0$, we would have

$$P_{ij}(\vec{x},t) = P(\vec{x},t)\delta_{ij} = -\frac{D}{2(t+t_0)}\rho(\vec{x},t)\delta_{ij} \quad (23)$$

for all $\vec{x} \in R^3$ and $t \geq 0$. Here $\delta_{ij}$ stands for the Kronecker symbol. Then, $-\int_V \rho\vec{\nabla}Q d^3x = -\int_{\partial V} P d\vec{\sigma}$, where

$$Q(\vec{x},t) = \frac{\vec{x}^2}{8(t+t_0)^2} - \frac{3D}{2(t+t_0)} \ . \quad (24)$$

The current velocity $\vec{v}(\vec{x},t) = \vec{\nabla}S(\vec{x},t) = \frac{\vec{x}}{2(t+t_0)}$, apart from solving $\partial_t\rho = -\vec{\nabla}\cdot(\vec{v}\rho)$ and $\partial_t\vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v} = -\vec{\nabla}Q$ with $\rho_0$ and $\vec{v}_0 = -\vec{u}_0$ standing for initial data, is also linked to the Hamilton-Jacobi equation

$$\partial_t S + \frac{1}{2}|\vec{\nabla}S|^2 + Q = 0 \quad (25)$$

whose solution is: $S(\vec{x},t) = \frac{\vec{x}^2}{4(t+t_0)} + \frac{3}{2}Dln[4\pi D(t+t_0)]$.

Let us observe that the initial data $\vec{v}_0 = -D\vec{\nabla}ln\,\rho_0 = -\vec{u}_0$ for the current velocity field indicate that we have totally ignored a crucial *preliminary* stage of the dynamics on the $\beta^{-1}$ time scale, when the Brownian expansion of an initially *static* ensemble has been ignited and so particles have been ultimately set in motion.

Notice also that our "osmotic expansion pressure" $P(\vec{x},t)$ is not positive definite, in contrast to the familiar kinetic theory (equation of state) expression for the pressure $P(\vec{x}) = \alpha\,\rho^\beta(\vec{x})$, $\alpha > 0$ appropriate for gases. The admissibility of the negative sign of the "pressure" function encodes the fact that the Brownian evolving concentration of particles generically decompresses (blows up), instead of being compressed

by the surrounding medium. The compression (pressure upon the control volume coming from its surrounding) is the standard feature in the kinetic theory of gases, except for the cavitation phenomenon in liquids and the exotic blow-up conditions in the concentrations of dense hot matter.

The loss (in view of the "osmotic" migration) of momentum stored in a control volume at a given time, may be here interpreted in terms of an acceleration $-\int_V \rho\vec{\nabla}Qd^3x$ induced by a *fictituous* "attractive force". By invoking an explicit Hamilton-Jacobi connection (21), we may attribute to a diffusing Brownian ensemble floating through a (locally co-moving) control volume $V$, the mean kinetic energy per unit of mass $\int_V \rho\frac{1}{2}\vec{v}^2d^3x$. We can also evaluate the mean total kinetic energy per unit of mass obtained after extending integrations from $V$ to $R^3$.

For the considered example, in view of $<\vec{x}^2>=6D(t+t_0)$, we have $\int_{R^3}\rho\frac{1}{2}\vec{v}^2d^3x=\frac{3D}{4(t+t_0)}$. Notice that the mean energy $\int_V\rho(\frac{1}{2}\vec{v}^2+Q)d^3x$ needs not to be positive. Indeed, this expression identically vanishes after extending integrations from $V$ to $R^3$. On the other hand the kinetic contribution, initially equal $\int_{R^3}\frac{1}{2}\rho v^2d^3x=3D/\alpha^2$ and evidently coming from nowhere, continually diminishes and is bound to disappear in the asymptotic $t\to\infty$ limit, when Brownian particles become uniformly distributed in space.

## 3.2 The third Newton law in the mean and the Brownian recoil principle

Normally, diffusion processes yielding a nontrivial matter transport (diffusion currents) are observed for a non-uniform concentration of colloidal particles. We can devise a thought (numerical) experiment that gives rise to a corresponding transport in terms of an ensemble of sample Brownian motion realisations on a fixed finite time interval, instead of considering a multitude of them (migrating swarm of Brownian particles) simultaneously. One may surely implant particles at initial (random) space locations to mimic a certain probability density and next release

(individually in each sample experiment) and allow them to execute their Brownian paths independently, in a fixed duration time interval. In terms of such a particle ensemble, we can safely return back to the previous colloidal diffusion picture where migrating Brownian particles are also regarded as independent (and so are their individual Brownian motions).

Consequently, in both visualizations, after the relaxation time $\beta^{-1}$, the diffusion current is initiated "at the expense" of the bath. A nonzero mean kinetic energy must have been initially transferred (pumped) from the bath to the diffusing (blowing-up, expanding) swarm of particles. Only asymptotically this energy is being returned back to the bath.

Recalling our previous discussion, for a sufficiently fast diffusion process, all that should correspond to a local cooling of the bath and implement a tiny deviation from its thermal equilibrium conditions in each single particle propagation (simulation) experiment. Accordingly, the tendency to regain the local thermal equilibrium by the bath (reflecting an attraction of tagged particles by the cooler areas) must result in induced local flows - they can become identifiable only on the ensemble average. All that is to happen *not* literally on the $\beta^{-1}$ relaxation time scale but on (still relatively small) time scale $\triangle t$ of the diffusion process which is well below the observational one.

To each executed sample path there corresponds a sample realisation of the random medium (pushed slightly away from its thermal equilibrium, in view of the postulated feedback mechanism). Those random (sample) realisations of the bath should be ensemble-averaged as well to yield an "effective" bath in thermal equlibrium, which is however no longer in a statistical state of rest. The emergent driving flows mimic, on the average, the "return to equilibrium" of the bath in each sample propagation experiment. The thermal conditions are maintained on the ensemble average, so that the *effective* process guiding the *ensemble* dynamics can be viewed as isothermal.

We recall close links of this scenario with an idea of a random walk in a random medium, [18]. However, presently a disorder in the random medium is coupled to the randomness of the walk and is no longer of independent origin.

Let us assume that "an effort" (hence, an energy loss) of the random medium, on the $\beta^{-1}$ scale, to produce a local Brownian diffusion current $\vec{v}(\vec{x}, t_0)$ out of the initially static ensemble and thus to decompress (lower the blow-up tendency) an initial non-uniform probability distribution, results in the *effective osmotic reaction* of the random medium. Whatever is being transported away (on the ensemble average) according to the Fick law, is assumed to induce a compensating osmotic counterflow in the *effective thermal bath.* That is the Brownian recoil effect of Ref. [11].

Now, the particle swarm propagation scenario becomes entirely different from the standard one, (10), (20). First of all, the nonvanishing forward drift $\vec{b} = \vec{u}$ is generated as a dynamical (effective, statistical here !) response of the bath to the enforced by the bath particle transport with the local velocity $\vec{v} = -\vec{u}$. Second, we need to account for a parellel inversion of the pressure effects (compression $+\vec{\nabla}Q$ should replace the decompression $-\vec{\nabla}Q$) in the respective local momentum conservation law.

Those features can be secured through an explicit realization of the action-reaction principle ("the Brownian recoil" effect, cf. Ref. [11]), which we promote to the status of the *third Newton law in the mean.*

On the level of Eq. (10), once averaged over a finite volume, we interpret the momentum per unit of mass rate-of-change $\int_V \rho\vec{\nabla}(\Omega - Q)d^3x$ which occurs exclusively due to the Brownian expansion, to generate a counterbalancing rate-of-change tendency in the random medium. To account for the emerging forward drift and an obvious modification of the subsequent dynamics of an ensemble of (tagged) particles, we re-define Eq. (10) by setting $-\int_V \rho\vec{\nabla}(\Omega - Q)d^3x$ in its right-hand-side instead of $+\int_V \rho\vec{\nabla}(\Omega - Q)d^3x$ . That amounts to an instantaneous realisation of

the third Newton law in the mean (action-reaction principle). Hence, the momentum conservation law for the process *with a recoil* (the reaction term replaces the decompressive "action" term) would read:

$$\partial_t \vec{v} + (\vec{v} \cdot \vec{\nabla})\vec{v} = \vec{\nabla}(Q - \Omega) \tag{26}$$

implying that

$$\partial_t S + \frac{1}{2}|\vec{\nabla} S|^2 - Q = -\Omega \tag{27}$$

stands for the corresponding Hamilton-Jacobi equation, cf. [19, 24], instead of Eq. (21). A suitable adjustment (re-setting) of the initial data is here necessary, which we shall explain in below (cf. Section 3.3).

The major idea of the Brownian motion with a recoil is thus given.

In the coarse-grained picture of motion we shall deal with a sequence of repeatable scenarios realised on the Smoluchowski process time scale $\triangle t$: the Brownian swarm expansion build-up is accompanied by the parallel counterflow build-up, which in turn modifies the subsequent stage of the Brownian swarm migration (being interpreted to modify the forward drift of the process) and the corresponding built-up anew counterflow.

Although the new closed system of partial differential equations (20) and (27) is very different from the previous one (20), (21), nonetheless it describes Markovian diffusion-type processes again, [2, 12, 25]. The link is particularly obvious if we observe that the new Hamilton-Jacobi equation (27) can be formally rewritten in the previous form (21) by introducing:

$$\Omega_r = \partial_t S + \frac{1}{2}|\vec{\nabla} S|^2 + Q$$

$$\Omega_r = 2Q - \Omega \tag{28}$$

where $\Omega$ represents the previously defined potential function of any Smoluchowski (or more general) diffusion process, (11). It is $\Omega_r$ which via Eq. (17) would determine

forward drifts of the Markovian diffusion process with a recoil. They must obey the Cameron-Martin-Girsanov identity

$$\Omega_r = 2Q - \Omega = 2D[\partial_t \phi + \frac{1}{2}(\frac{\vec{b}^2}{2D} + \vec{\nabla} \cdot \vec{b})] \ . \tag{29}$$

Our system of equations (20), (27) is badly nonlinear and coupled, but its linearisation can be immediately given in terms of an adjoint pair of Schrödinger equations with a potential $\Omega$, [2, 19]. Indeed,

$$i\partial_t \psi = -D\triangle\psi + \frac{\Omega}{2D}\psi \tag{30}$$

with a solution

$$\psi = \rho^{1/2} exp(iS) \tag{31}$$

and its complex adjoint makes the job, if we regard $\rho$ together with $S$ to remain in conformity with the previous notations of Eqs. (20), (27). The choice of $\psi(\vec{x}, 0)$ gives rise to a solvable Cauchy problem. This feature we shall exploit in below. Notice that, in view of Eq. (30), for time-indepedent $\Omega$, the total energy $\int_{R^3}(\frac{v^2}{2} - Q + \Omega)\rho d^3x$ of the diffusing ensemble is a conserved quantity.

The problem (20), (27), (28) can be reformulated as the Schrödinger boundary data problem (cf. the Appendix), but the resulting generalised diffusion equations are nonlinearly coupled (by means of the potential $\Omega_r$ replacing the Feynman-Kac potential $\Omega$. Hence the previous linearisation needs to be exploited anyway. The general existence criterions for Markovian diffusion processes of that kind, were formulated in Ref. [25], see also [19, 12] and the Appendix.

## 3.3 Brownian motion with a recoil as an anomalous (enhanced) diffusion model

For the clarity of discussion, we shall confine our considerations to one-dimensional problems. In the absence of external forces, we may consider a solution of equations (in space dimension one) $\partial_t \rho = -\nabla(v\rho)$ and $\partial_t v + (v\nabla)v = +\nabla Q$, where an

initial probability density $\rho_0(x)$ is chosen in correspondence with the previous free Brownian motion example. We denote $\alpha^2 = 4Dt_0$. Then,

$$\rho(x,t) = \frac{\alpha}{[\pi(\alpha^4 + 4D^2t^2)]^{1/2}}\, exp[-\frac{x^2\alpha^2}{\alpha^4 + D^2t^2}] \tag{32}$$

and

$$b(x,t) = v(x,t) + u(x,t) = \frac{2D(\alpha^2 - 2Dt)x}{\alpha^4 + 4D^2t^2} \tag{33}$$

are the pertinent solutions. Notice that $u(x,0) = -\frac{2Dx}{\alpha^2} = b(x,0)$ amounts to $v(x,0) = 0$, while in the previous free Brownian case the initial current velocity was equal to $-D\nabla ln\,\rho_0$. This re-adjustment of the initial data can be interpreted in terms of the counterbalancing (recoil) phenomenon: the would-be initial Brownian ensemble current velocity $v_0 = -u_0$ is here completely saturated by the emerging forward drift $b_0 = u_0$, see e.g. also [11]. This implies $u(x,t) = -\frac{2D\alpha^2 x}{\alpha^4+4D^2t^2}$ and $v(x,t) = \frac{4D^2xt}{\alpha^4+4D^2t^2}$. Notice that $\nabla Q = \frac{x\alpha^4}{4(\alpha^4+D^2t^2)}$, to be compared with the respective expression $-\vec{\nabla}Q = -\frac{D^2x}{\alpha^2+4Dt}$ in the previous section. Presently, we deal with a fictituous "repulsive" force, which corresponds to the compression (pressure upon) of the Brownian ensemble due to the counter-reaction of the surrounding medium.

We can write things more explicitly. Namely, now:

$$Q(x,t) = \frac{2D^2\alpha^2}{\alpha^4 + 4D^2t^2}(\frac{\alpha^2x^2}{\alpha^4 + 4D^2t^2} - 1) \tag{34}$$

and the corresponding pressure term ($\nabla Q = \frac{1}{\rho}\nabla P$) reads

$$P(x,t) = -\frac{2D^2\alpha^2}{\alpha^4 + 4D^2t^2}\rho(x,t) \tag{35}$$

giving a positive contribution $+\nabla Q$ to the local conservation law (26).

The related Hamilton-Jacobi equation

$$\partial_t S + \frac{1}{2}|\nabla S|^2 = +Q \tag{36}$$

is solved by

$$S(x,t) = \frac{2D^2x^2t}{\alpha^4 + 4D^2t^2} - D\,arctan\,(-\frac{2Dt}{\alpha^2}) \tag{37}$$

With the above form of $Q(x,t)$ one can readily check that equations (28) are identically satisfied, and that the Cameron-Martin-Girsanov constraint euqation for the forward drift of the Markovian diffusion process with a recoil is automatically valid for $\phi = \frac{1}{2} ln\, \rho + S$:

$$2Q = 2D[\partial_t \phi + \frac{1}{2}(\frac{b^2}{2D} + \nabla \cdot b)] \tag{38}$$

cf. the general identity (29).

In anology with our free Brownian motion discussion, let us observe that presently

$$< x^2 >= \frac{\alpha^2}{2} + \frac{2D^2 t^2}{\alpha^2} \ . \tag{39}$$

It is easy to demonstrate (use a linearisation (30), (31) of the problem) that the quadratic dependence on time persists for arbitrarily shaped initial choices of the probability distribution $\rho_0(x) > 0$. That signalizes an anomalous behaviour (enhanced diffusion) of the pertinent Markovian process when $\Omega = 0$ i. e. $\Omega_r = 2Q$.

We can evaluate the kinetic energy contribution

$$\int_R \rho \frac{v^2}{2} dx = \frac{4D^4 t^2}{\alpha^2(\alpha^4 + 4D^2 t^2)} \tag{40}$$

which in contrast to the Brownian case shows up a continual growth up to the terminal (asymptotic) value $\frac{D^2}{\alpha^2}$. This value was in turn an initial kinetic contribution in the previous Brownian example. In contrast to that case, the total energy integral is now finite (finite energy diffusions of Ref. [25]) and reads

$$\int_R (\frac{1}{2} v^2 - Q)\rho dx = \frac{D^2}{\alpha^2} \tag{41}$$

for all times (it is a conservation law). The asymptotic value of the current velocity $v \sim \frac{x}{t}$ is twice larger than this appropriate for the Brownian motion, $v \sim \frac{x}{2t}$.

## 3.4 Response to an external force: non-dispersive diffusion-type processes

Let us regard $\vec{F}(\vec{x}) = -\vec{\nabla} V(\vec{x})$ as an external force field, whose effects on the dynamics of Brownian particles is encoded in the Smoluchowski diffusion process

equations (7), (9) and next (9)-(11). Those in turn can be motivated by invoking the Kramers equation (14) and its Smoluchowski diffusion approximation (15).

As emphasized before, on the level of local conservation laws, in the diffusion approximation, the microscopic force $\vec{F}$ is represented by the (Feynman-Kac) potential $\Omega$, defined through the Girsanov formula (11).

Let us adopt the third Newton law in the mean and the related Brownian recoil strategy (26)-(29) to this case. Evidently, the potential $\Omega$ will explicitly appear in the linearization (30) of the problem. On the other hand, it is the potential $\Omega_r = 2Q - \Omega$ which via Eq. (29) determines forward drifts appropriate for the diffusion process with a recoil. In view of an inherent nonlinearity of the problem, one should not expect that the emergent drifts would allow for a simple decomposition met in Eqs. (14), (15).

Our further discussion will be carried out in one space dimension and will focus on quadratic potentials.

For a parabolic (harmonic oscillator) potential $V(x) = \frac{1}{2}m\omega^2 x^2$ defining the acceleration $K(x) = -\omega^2 x$, the corresponding Feynman-Kac potential (11) reads $\Omega(x) = \frac{1}{2}\gamma^2 x^2 - D\gamma$, $\gamma = \frac{\omega^2}{\beta}$. It is useful to mention that the choice of the repulsive potential $V(x) = +\frac{1}{2}m\omega^2 x^2$ would yield an innocent-looking modification by a constant in the function (17): $\Omega(x) = \frac{1}{2}\gamma^2 x^2 + D\gamma$. That demonstrates an extraodrinary sensitivity of the Riccatti-type equations (11) and (17) on the choice of $\Omega$.

In fact, a suitable additive modification of $\frac{1}{2}\gamma^2 x^2$ by a constant, allows to generate (by directly solving the Riccatti-type equation (11)) the whole family of forward drifts pertaining to *inequivalent* stationary diffusion processes, cf. [12]. Nonetheless, all of them correspond to the same $\nabla\Omega = +\gamma^2 x$ generic contribution to the local momentum conservation law (10). Clearly, the law (10) does not provide a sufficiently fine discrimination between admissible stochastic motion scenarios, unless we know the Smoluchowski force and its potential from the beginning. It is only the Hamilton-Jacobi equation level, where the closed system of partial differential

equations (respectively (20), (21) or (20), (27)) determines the process uniquely.

It is clear that stationary processes *are the same* both in case of the standard Brownian motion and the Brownian motion with a recoil. The respective propagation scenarios substantially differ in the non-stationary case only.

To exemplify the above statement (we have discussed before the $\Omega = 0$ case), let us consider an explicit solution of Eqs. (20) and (28) in case of $\Omega(x) = \frac{1}{2}\gamma^2 x^2 - D\gamma$. By means of the linearisation (30), (31), this can be easily accomplished, cf. [24]. We shall utilse exactly the same inital probability density $\rho_0(x)$ as before. We have:

$$\rho(x,t) = [\frac{\gamma\alpha^2}{\pi(sin^2(\sqrt{\gamma}2Dt) + \gamma\alpha^4 cos^2(\sqrt{\gamma}2Dt))}]^{1/2}\cdot$$

$$\cdot exp[-\frac{\gamma\alpha^2 x^2}{sin^2(\sqrt{\gamma}2Dt) + \gamma\alpha^4 cos^2(\sqrt{\gamma}2Dt)}] \tag{41}$$

and

$$S(x,t) = -\frac{D(\gamma)^{3/2}\alpha^4 x^2 tg\,(\sqrt{\gamma}2Dt)}{(tan^2(\sqrt{\gamma}2Dt + \gamma\alpha^4)sin(\sqrt{\gamma}2Dt)} + \frac{D\sqrt{\gamma}x^2}{tan(\sqrt{\gamma}2Dt)} +$$

$$+Darctan\,[-\frac{tan(\sqrt{\gamma}2Dt)}{\sqrt{\gamma}\alpha^2}] - D\gamma t\ . \tag{42}$$

The forward drift of the corresponding diffusion-type process reads:

$$b(x,t) = \frac{(1-\gamma\alpha^2)\sqrt{\gamma}sin(\sqrt{\gamma}4Dt) - 2\gamma\alpha^2}{sin^2(\sqrt{\gamma}2Dt) + \gamma\alpha^4 cos^2(\sqrt{\gamma}2Dt)}Dx \tag{43}$$

and $X(t) = x$ holds true in terms of the random variable of the process. The additive decomposition of the drift, valid in Eqs (9), (15), is completely destroyed by the Brownian recoil scenario. Notice that $b(x,0) = -\frac{2Dx}{\alpha^2} = u(x,0)$, while (cf. (9)) $b = \frac{F}{m\beta} = -\gamma x$ would hold true for all times, in case of the standard Smoluchowski diffusion process.

Because of the harmonic attraction and suitable initial probability measure choice, we have here wiped out all previously discussed enhanced diffusion features. Now, the dispersion is attentuated and actually the non-dispersive diffusion-type

process is realised: $< x^2 >$ does not spread at all despite of the intrinsically stochastic nature of the dynamics (finite-energy diffusions of Ref. [25]).

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## Appendix: Reconstruction of a Markovian diffusion process from the input-output statistics data

There are many procedures to reproduce the intrinsic dynamics of a physical system from observable data, like e.g. the time series analysis. We shall outline an algorithm allowing to reconstruct the *most likely* microscopic motion scenario under an additional assumption that the sought for dynamics actually *is* a Markovian diffusion process. This reconstruction method is based on solving the so-called Schrödinger boundary-data and interpolation problem, [19, 12, 23].

Given two strictly positive (usually on an open space-interval) boundary probability densities $\rho_0(\vec{x}), \rho_T(\vec{x})$ for a process with the time of duration $T \geq 0$. One can single out a unique Markovian diffusion process which is specified by solving the Schrödinger boundary data problem:

$$m_T(A,B) = \int_A d^3x \int_B d^3y \, m_T(\vec{x},\vec{y})$$

$$\int d^3y \, m_T(\vec{x},\vec{y}) = \rho_0(\vec{x})$$

$$\int d^3x \, m_T(\vec{x},\vec{y}) = \rho_T(y)$$

where the joint probability distribution has a density

$$m_T(\vec{x},\vec{y}) = u_0(\vec{x}) \, k(x,0,y,T) \, v_T(\vec{y})0$$

and the two unknown functions $u_0(\vec{x})$, $v_T(\vec{y})$ come out as (unique) solutions, of *the same sign,* of the integral identities. To this end, we need to have at our disposal a continuous bounded strictly positive (ways to relax this assumption are known) function $k(\vec{x}, s, \vec{y}, t), 0 \leq s < t \leq T$, which for our purposes (an obvious way to secure the Markov property) is chosen to be represented by familiar Feynman-Kac integral kernels of contractive dynamical semigroup operators:

$$k(\vec{y}, s, \vec{x}, t) = \int exp[-\int_s^t c(\vec{\omega}(\tau), \tau) d\tau] d\mu_{(\vec{x},t)}^{(\vec{y},s)}(\omega)$$

The pertinent (interpolating) Markovian process can be ultimately determined by means of positive solutions (it is desirable to have them bounded) of the adjoint pair of generalised heat equations:

$$\partial_t u(\vec{x}, t) = \nu \triangle u(\vec{x}, t) - c(\vec{x}, t) u(\vec{x}, t)$$

$$\partial_t v(\vec{x}, t) = -\nu \triangle v(\vec{x}, t) + c(\vec{x}, t) v(\vec{x}, t) \ .$$

Here, a function $c(\vec{x}, t)$ is restricted only by the positivity and continuity demand for the kernel. In the above, $d\mu_{(\vec{x},t)}^{(\vec{y},s)}(\omega)$ is the conditional Wiener measure over sample paths of the standard Brownian motion.

Solutions, upon suitable normalisation give rise to the Markovian diffusion process with the *factorised* probability density $\rho(\vec{x}, t) = u(\vec{x}, t) v(\vec{x}, t)$ which, while evolving in time, interpolates between the boundary density data $\rho(\vec{x}, 0)$ and $\rho(\vec{x}, T)$. The interpolation admits an Itô realisation with the respective forward and backward drifts defined as follows:

$$\vec{b}(\vec{x}, t) = 2\nu \frac{\nabla v(\vec{x}, t)}{v(\vec{x}, t)}$$

$$\vec{b}_*(\vec{x}, t) = -2\nu \frac{\nabla u(\vec{x}, t)}{u(\vec{x}, t)}$$

in the prescribed time interval $[0, T]$.
For the forward interpolation, the familiar Fokker-Planck (second Kolmogorov) equation holds true:

$$\partial_t \rho(\vec{x}, t) = \nu \triangle \rho(\vec{x}, t) - \nabla[\vec{b}(\vec{x}, t) \rho(\vec{x}, t)]$$

with $\rho(\vec{x},0)$ given, while for the backward interpolation (starting from $\rho(\vec{x},T)$) we have:

$$\partial_t\rho(\vec{x},t) = -\nu\triangle\rho(\vec{x},t) - \nabla[\vec{b}_*(\vec{x},t)\rho(\vec{x},t)] \ .$$

The drifts are gradient fields, $curl\,\vec{b} = 0$. As a consequence, those that are allowed by any prescribed choice of the function $c(\vec{x},t)$ *must* fulfill the compatibility condition

$$c(\vec{x},t) = \partial_t\Phi \ + \ \frac{1}{2}(\frac{b^2}{2\nu} + \nabla b)$$

which establishes the Girsanov-type connection of the forward drift $\vec{b}(\vec{x},t) = 2\nu\nabla\Phi(\vec{x},t)$ with the Feynman-Kac potential $c(\vec{x},t)$. In the considered Schrödinger's interpolation framework, the forward and backward drift fields are connected by the identity $\vec{b}_* = \vec{b} - 2\nu\nabla ln\rho$.

For Markovian diffusion processes the notion of the *backward* transition probability density $p_*(\vec{y},s,\vec{x},t)$ can be consistently introduced on each finite time interval, say $0 \leq s < t \leq T$:

$$\rho(\vec{x},t)p_*(\vec{y},s,\vec{x},t) = p(\vec{y},s,\vec{x},t)\rho(\vec{y},s)$$

so that $\int \rho(\vec{y},s)p(\vec{y},s,\vec{x},t)d^3y = \rho(\vec{x},t)$ and $\rho(\vec{y},s) = \int p_*(\vec{y},s,\vec{x},t)\rho(\vec{x},t)d^3x$.

The transport (density evolution) equations refer to processes running in opposite directions in a fixed, common for both time-duration period. The forward one executes an interpolation from the Borel set $A$ to $B$, while the backward one executes an interpolation from $B$ to $A$.

The knowledge of the Feynman-Kac kernel implies that the transition probability density of the forward process reads:

$$p(\vec{y},s,\vec{x},t) = k(\vec{y},s,\vec{x},t)\frac{v(\vec{x},t)}{v(\vec{y},s)} \ .$$

while the corresponding transition probability density of the backward process has the form:

$$p_*(\vec{y},s,\vec{x},t) = k(\vec{y},s,\vec{x},t)\frac{u(\vec{y},s)}{u(\vec{x},t)} \ .$$

Obviously in the time interval $0 \leq s < t \leq T$ there holds:

$$u(\vec{x},t) = \int u_0(\vec{y}) k(\vec{y},s,\vec{x},t) d^3y$$

$$v(\vec{y},s) = \int k(\vec{y},s,\vec{x},T) v_T(\vec{x}) d^3x \ .$$

Consequently, we have fully determined the underlying (Markovian) random motions, forward and backward, respectively. All that accounts for perturbations of (and conditioning upon) the Wiener noise.

**Remark 6:** Various partial differential equations associated with Markovian diffusion processes are known *not* to be invariant under time reversal (hence being dissipative and linked to irreversible physical phenomena). However, the correspoding processes admit a *statistical inversion.* Let us consider a process running in a finite time interval, say $[0,T]$. We may consistently define a process running backward in time in this interval and reproducing the most likely (statistical) past of the process, given the present probability measure data. See e.g. [2, 11, 12, 19] and [26]. In fact, cf. [27] p. 255: " any probabilistic treatement of the heat equation involves a time-reversal". This feature is explicitly utilized in the analysis of the above outlined Schrödinger boundary-data and interpolation problem, [19, 12].

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